The 2nd ISSP-MPIPKS Joint Workshop

Dynamics of Strongly Correlated Systems

March 30–31, 2015

Main Lecture Hall of the Institute for Solid State Physics, The University of Tokyo

Mar 30 (Mon)

10:00 – 10:05 Opening address (Masashi Takigawa, Director of ISSP)

10:05 – 10:15 ISSP and MPI-PKS (Kazuo Ueda, Former director of ISSP)

Topological state, entanglement, and correlation

10:15 – 10:55 Frank Pollmann* (Max-Planck-Institut für Physik komplexer Systeme)
Entanglement, and dynamics in many-body localized systems

10:55 – 11:35 Masaki Oshikawa* (The Institute for Solid State Physics)
Symmetry protection of critical phases and global anomaly in 1+1 dimensions

11:35 – 12:15 Toshikaze Kariyado (University of Tsukuba)
Correlation effects on the topological edge states in graphene nanoflakes: Relation between nanostructure and local magnetic order

12:15 – 13:30 lunch

Nonequilibrium Mott physics and charge properties

13:30 – 14:10 Ichiro Terasaki* (Nagoya University)
The Mott insulator Ca_2RuO_4 in a non-equilibrium steady state

14:10 – 14:50 Akira Ueda* (The Institute for Solid State Physics)
Hydrogen-bonded purely organic conductors: Exploration of hydrogen-bond-dynamics-coupled electronic properties

14:50 – 15:05 break

Dynamics in frustrated systems

15:05 – 15:45 Mathieu Taillefumier* (Okinawa Institute of Science and Technology)
Semi-classical spin dynamics of the antiferromagnetic Heisenberg model on the kagome lattice

15:45 – 16:25 Masafumi Udagawa* (The University of Tokyo)
Emergent collective excitations and anomalous dynamics of spin ice with short-range interaction

16:25 – 17:50 poster session

18:00 – 20:00 banquet

Mar 31 (Tue)

QCP and topological phases

9:00 – 9:40 Yosuke Matsumoto* (The Institute for Solid State Physics)
Emergent critical phase in a correlated electron system

9:40 – 10:20 Tsuneya Yoshida (RIKEN)
Classification of two-dimensional symmetry protected topological phases with a reflection symmetry

10:20 – 10:35 break

Quantum spin ice

10:35 – 11:15 Kenta Kimura* (Osaka University)
Quantum fluctuations in exchange-based spin ice $Pr_2Zr_2O_7$

11:15 – 11:55 Olga Petrova* (Max-Planck-Institut für Physik komplexer Systeme)
Magnetic monopoles in diluted quantum spin ice

11:55 – 13:20 lunch

Skyrmion and Higgs mode

13:20 – 14:00 Naoto Nagaosa* (RIKEN and The University of Tokyo)
Dynamics of coupled electrons, skrymions and monopoles

14:00 – 14:40 Naoto Tsuji (The University of Tokyo)
Light-induced Higgs-mode resonance in s-wave and d-wave superconductors

14:40 – 14:55 break

Quantum spin liquids

14:55 – 15:35 Yoshitomo Kamiya* (RIKEN)
Solidifying a quantum spin liquid in a 3D toric code

15:35 – 16:15 Dima Kovrizhin* (University of Cambridge)
Dynamics in quantum spin-liquids

16:15 – 16:20 Closing address (Hirokazu Tsunetsugu, ISSP)

(*: invited speakers)

Poster session

PS-01 Koudai Iwahori (Kyoto University)
Periodically-driven Kondo impurity coupled to an ultracold fermionic bath

PS-02 Masaya Nakagawa (Kyoto University)
Photo-induced Kondo effect and its anomalous behavior

PS-03 Akihisa Koga (Tokyo Institute of Technology)
Transport properties for a quantum dot coupled to normal leads with the pseudogap structure

PS-04 Yuta Murakami (The University of Tokyo)
Dynamical mean-field analysis of non-equilibrium relaxation processes
in an electron-phonon coupled system

PS-05 Takumi Ohta (Yukawa Institute for Theoretical Physics)
Phase diagram of a one-dimensional generalized cluster model and dynamics
during an interaction sweep

PS-06 Yuya Nakagawa (The Institute for Solid State Physics)
Flux quench in the S=1/2 XXZ chain

PS-07 Kazuaki Takasan (Kyoto University)
Topological Kondo insulators in strong laser fields

PS-08 Satoru Maeda (Kyushu Institute of Technology)
Effect of Ca-doping on pyrochlore iridates $Nd_2Ir_2O_7$

PS-09 Kim Hyeon-Deuk (Kyoto University)
Dynamical analyses of condensed-phase hydrogens using nuclear
and electron wave packet molecular dynamics simulation

PS-10 Tomoyuki Hamada (Hitachi Ltd.)
First principle calculation of electronic structures of lantanide oxides
with pseudopotential method

PS-11 Takeru Nakayama (The Institute for Solid State Physics)
Fano resonance between Higgs bound states and Nambu-Goldstone modes

PS-12 Katsuaki Kobayashi (University of Electro-Communications)
Convergence for the groundstate auxiliary field method

PS-13 Amane Uehara (The University of Tokyo)
Theoretical study of charge-spin-orbital fluctuations in mixed valence spinels:
AlV_2O_4 and LiV_2O_4

PS-14 Yusuke Sugita (The University of Tokyo)
Excitonic multipole order in a d-p model with parity mixing

PS-15 Joji Nasu (Tokyo Institute of Technology)
Finite temperature phase transition in chiral spin liquids

PS-16 Takanori Sugimoto (Tokyo University of Science)
Magnetization process in a frustrated spin ladder

PS-17 Kazuhiko Tanimoto (Yukawa Institute for Theoretical Physics)
Topological quantum phase transition in an SU(N)-invariant spin chain

PS-18 Ryo Ozawa (The University of Tokyo)
Meron crystals with spin scalar chiral stripes

PS-19 Hiroyuki Fujita (The Institute for Solid State Physics)
Chiral magnetic effect in insulators

Oral Presentations

Entanglement and dynamics in Many-Body Localized Systems

R. Singh[1], J. Kjäll[2], J. H. Bardarson [1], F. Pollmann[1]

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Many-body localized (MBL) phases occur in isolated quantum systems when Anderson localization persists in the presence of finite interactions. It turns out that the entanglement is a very useful quantity to study these phases. First, we use the bipartite entanglement of excited eigenstates to pinpoint a phase transition from a localized to an extended phase in a random Ising chain with short ranged interactions [1]. A characterizing property of the MBL phase is that the area law also applies to excited states. Thus, in one-dimensional systems, these states can be encoded efficiently using a matrix-product state representation. Second, we study the time evolution of simple (unentangled) initial states for a system of interacting spinless fermions in a one dimensional system. It is found that interactions induce a dramatic change in the propagation of entanglement.

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Symmetry protection of critical phases and global anomaly in $1+1$ dimensions

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Classification of quantum phases is a central problem in condensed matter and statistical physics. They can be first classified into gapped and gapless phases. Gapped quantum phases are relatively easier to be handled theoretically. In fact, there has been a significant progress in further classification of gapped phases. In particular, symmetry protected topological (SPT) phases has become an important concept in the classification [1]. That is, even when two states have no long-range entanglement and are indistinguishable in terms of any local observables, in the presence of a certain symmetry, they could still belong to distinct phases separated by a quantum phase transition.

In contrast, classification of gapless quantum phases remains very much open. Symmetries are naturally expected to play an important role also in the classification of gapless quantum phases. Interestingly, symmetry protection of gapless quantum phases has been better understood for the gapless edge states of SPT phases. As a simple and well-known example, the helical edge state of a topological insulator remains gapless even in the presence of impurities, as long as the system is time-reversal invariant. This indeed leads to the stability of the topological insulator as an SPT phase in the presence of the time-reversal symmetry. This approach is recently refined and generalized in terms of anomaly [2]. In short, the edge state of an SPT phase exhibits an anomaly with respect to the relevant symmetry, which implies the "ingappability" of the edge state in presence of the symmetry. This also motivates us to question if there is a mechanism of symmetry protection of the universality class of *bulk* gapless critical phases.

In this talk, we argue that there is a protection of bulk gapless critical phases by discrete symmetry. This symmetry protection is quite analogous to that of the well-known (gapped) SPT phases; here we show that the concept can be generalized to bulk *gapless critical* phases. We demonstrate this for the SU(2)-symmetric quantum antiferromagnetic chains and their effective field theory, SU(2) Wess-Zumino-Witten (WZW) theory as an example. The SU(2) WZW theory is characterized by a natural number k, which is called level. Hereafter we denote the level-k SU(2) WZW theory as $\mathrm{SU}(2)_k$ WZW theory. The $\mathrm{SU}(2)_k$ WZW theories with $k = 1, 2, \ldots$ are thought to be a complete classification of the universality classes of critical points in $1+1$ dimensions with the Lorentz and SU(2) symmetry. We can also identify the level $k = 0$ with the gapped state with a unique "disordered" ground state. In the presence of the SU(2) and a certain discrete Z_2 symmetry of the WZW theory, which corresponds to the translation symmetry of the spin chain, we find that a renormalization-group (RG) flow is possible between $\mathrm{SU}(2)_k$ and $\mathrm{SU}(2)_{k'}$ WZW theories only if $k \equiv k' \bmod 2$. That is, the gapless critical phases in $1+1$ dimension with the SU(2), the Z_2, and the Lorentz symmetries are classified into the two "symmetry-protected" categories: one corresponds to even levels and the other to odd levels. In terms of spin chain models, as long as the SU(2) spin-rotation and the lattice translation symmetries are unbroken (either explicitly or spontaneously), a spin chain with an integer S can only realize $\mathrm{SU}(2)_k$ WZW theory with an even k, while one with a half-odd-integer S can only realize $\mathrm{SU}(2)_k$ WZW theory with an odd k [3].

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Correlation Effects on the Topological Edge States in Graphene Nanoflakes: Relation between Nanostructure and Local Magnetic Order

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At the zigzag edge of graphene, topologically protected edge states appear [1,2]. Correlation effects on this edge states are important since they form a flat band in the momentum space, which is prone to exhibits magnetic[1,3] or possibly some other kinds of order.

In this study, graphene nanoflakes with zigzag edges are theoretically studied focusing on the correlation effects on the edge states. A nanoflake is suitable to study relation between nanostructures and correlation effects. We first show that it is possible to have insights into edge states by constructing given flakes by cutting and pasting triangle flakes. A triangle flake with zigzag edges is an ideal "building block" since it has exact zero energy edge states. In numerics, the "cut and paste" is implemented as an adiabatic change of selected transfer integrals. By following the evolution of the energy levels and wave functions against this adiabatic change, insights on the edge states can be extracted. For instance, the suppression of the weight of edge state wave function at a 120° corner [4] can be understood by cutting a triangle. Similarly, 240° and 300° corners, are also investigated and it is shown that the edge states decrease at these corners. As a further application, we connect a shift in bulk Dirac cones caused by uniaxial strain and anisotoropy of the strained triangle flake by making graphene ribbon with triangles.

When the chiral symmetry exists, it sometimes becomes easy to handle correlation effects. That is, when the energy of the bulk states is far away from the zero energy edge states, it is possible to obtain an well approximated ground state wave function with the help of a pseudopotential by the chiral basis [5,6]. In some cases, including the case with the trinangle flake, the bulk states of nanoflakes have sizable gaps by finite size effect, and the idea becomes applicable. Then, we calculate the local spin moment induced by correlation using the obtained wave function. It is found that decrease of edge state at the corner has direct relevance to suppression of the local spin moment at the corner. Spatial resolution of the magnetic moment is beyond the Lieb's theorem for the total moment in chiral symmetric systems [7].

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The Mott insulator Ca_2RuO_4 in a non-equilibrium steady state

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The non-equilibrium steady state (NESS) is a steady state with constant flows of particle and energy. Obviously, it is the simplest system for non-equilibrium states, and many researchers have expected that the thermodynamics and statistical physics are able to be upgraded to include NESS. However, still missing is a real substance that exhibits essentially non-equilibrium characteristics.

Non-ohmic conduction is a typical example for NESS, and in particular we have focused on nonlinear conduction in strongly correlated electrons. As is generally agreed, strong correlation is a fertile source of electronic phase transitions such as high-temperature superconductivity in copper oxides, colossal magnetoresistance in manganese oxides, and multipole ordered states in heavy fermion intermetallics. Since some of such ordered states are susceptible to external impetus, we have searched for an ordered state susceptible to external electric field.

We have eventually arrived at the Mott insulator Ca_2RuO_4; this particular oxide undergoes a metal-insulator transition at around 360 K, and a low external pressure easily breaks the low-temperature insulating state. Nakamura et al. [1] have recently discovered a small electric field also breaks the insulating state. By controlling the sample temperature using black body radiation [2], we have observed the Seebeck coefficient in various external currents simultaneously. The resistivity decreases with increasing current density, and the Seebeck coefficient is significantly enhanced by 50-100 μV/K, which cannot be ascribed to a simple self heating. We have further found that the volume is changed with external current density in isothermal conditions.

In the present talk, we will show various anomalous properties of Ca_2RuO_4 in the nonlinear conduction regime, and compare them with those of other materials.

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Hydrogen-bonded Purely Organic Conductors: Exploration of Hydrogen-bond-dynamics-coupled Electronic Properties

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Hydrogen-bonded (H-bonded) organic conductors have attracted continuous attention because they show unique molecular arrangements, packing structures, and electronic (or electrostatic) features intrinsically due to the H-bond formation, resulting in various kinds of interesting physical properties and functionalities [1]. In these studies, the "static" effects of the H-bond are frequently used to control or regulate the crystal and electronic structures, however, the "dynamic" effects, such as proton (or hydrogen atom) transfer within the H-bond, on the electronic properties are little investigated.

We recently synthesized a new type of H-bonded purely organic conductor, κ-H_3(Cat-EDT-TTF)$_2$ (**κ-H**) [2], in which the conducting layers, composed of the Cat-EDT-$TTF^{+0.5}$ molecules, are directly connected by $[O\cdots H\cdots O]^{-1}$ H-bonds (Figure 1). This peculiar crystal structure, intrinsically different from that of the previous systems [1], has offered us an opportunity to explore novel electronic features and physical properties related to H-bond dynamics. In this presentation, I will firstly introduce the structure and properties of **κ-H** with a quantum spin liquid ground state [2, 3], and then give a detailed description about the $[O\cdots D\cdots O]^{-1}$ deuterated analogue, κ-D_3(Cat-EDT-TTF)$_2$ (**κ-D**), showing an unprecedented charge-order phase transition coupled to the H-bond dynamics [4], in terms of the H/D isotope and pressure effects.

This work was performed by collaboration with Mr. S. Yamada, Dr. T. Isono, Mr. H. Kamo, Prof. H. Mori (ISSP, The Univ. of Tokyo), Dr. A. Nakao (CROSS), Prof. R. Kumai, Prof. H. Nakao, Prof. Y. Murakami (KEK), Prof. K. Yamamoto (Okayama Univ. of Sci.), Prof Y. Nishio (Toho Univ.), and Prof. S. Uji (NIMS).

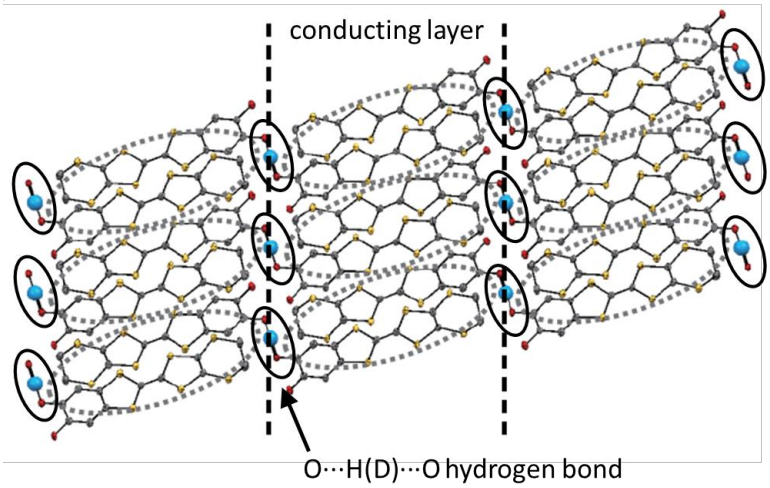

Figure 1: Crystal packing of **κ-H** and **κ-D**.

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Semi-classical spin dynamics of the antiferromagnetic Heisenberg model on the kagome lattice

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We investigate the dynamical properties of the classical antiferromagnetic Heisenberg model on the kagome lattice using a combination of Monte Carlo and molecular dynamics simulations. We find that frustration induces a distribution of timescales in the cooperative paramagnetic regime (*i.e.* far above the onset of coplanarity), as recently reported experimentally in deuterium jarosite. At lower temperature, when the coplanar correlations are well established, we show that the weathervane loop fluctuations control the system relaxation: the time distribution observed at higher temperatures splits into two distinct timescales associated with fluctuations in the plane and out of the plane of coplanarity. The temperature and wave vector dependences of these two components are qualitatively consistent with loops diffusing in the entropically dominated free energy landscape. Numerical results are discussed and compared with the $O(N)$ model and recent experiments for both classical and quantum realizations of the kagome magnets.

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Emergent collective excitations and anomalous dynamics of spin ice with short-range interaction

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Spin ice is a prototypical frustrated magnet, with a number of remarkable features, such as ground-state degeneracy, fractional excitations, and quasi-long range correlation, which now serve as fundamental concepts to understand frustrated magnetism. Among these properties, we focus on the dynamical character of spin ice. Indeed, $Ho(Dy)_2Ti_2O_7$, a canonical examples of dipolar spin ice system, exhibits several anomaly in its dynamics. It shows a drastic divergence of relaxation time at low temperatures [1, 2], and the role of monopole excitations in this extremely slow dynamics has been intensively discussed [3, 4]. Dynamical anomalies have also been found in several variants of spin ice. For example, in $Pr_2Ir_2O_7$, a metallic spin ice system, so-called spontaneous Hall effect has been observed [5], in possible relation to the slow dynamics of its compound at low temperatures.

In this contribution, we study the classical dynamics of J_1-J_2-J_3 spin ice model. This model is the simplest extension of the nearest-neighbor spin ice, and also captures the essential part of the metallic spin ice system, where conduction electrons interact with spin ice. Remarkably, this model can be mapped to the monopole gas model with the nearest-neighbor interaction on dual diamond lattice, if $J_2 = J_3 \equiv J$ is satisfied [6], and gives an idealistic test ground to study the effects of monopole interactions on dynamical properties.

We analyzed the classical dynamics of this model with a waiting-time Monte Carlo method, and clarified the time evolution of monopole density and magnetization for all the range of J. In particular, we found several quasi-stable macroscopic states survive as a steady state with macroscopically long relaxation time, even though they have higher energy compared with ground state. In this contribution, we will describe the nature of these steady states. In particular, we discuss the possible relation between the emergent collective excitation which we term "monopole jellyfish" and the spontaneous Hall effect observed in $Pr_2Ir_2O_7$ [7].

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Emergent critical phase in a correlated electron system

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In this talk, I would like to discuss the novel quantum criticality (QC) recently observed in the valence fluctuating $YbAlB_4$ systems. So far, QC in heavy fermion systems has been studied mainly for Kondo lattice systems with integer valence, where a quantum critical point is usually expected to be on the border of magnetism. On the other hand, the first Yb-based heavy fermion superconductor β-$YbAlB_4$ provides a unique example of QC in the mixed valent compounds [1, 2, 3, 4]. In addition, the QC cannot be explained by the standard spin fluctuation mechanism and emerges without tuning any control parameter, indicating formation of a strange metal phase [4]. Recent resistivity measurements under pressure have revealed that a non-Fermi liquid phase is stable over a finite pressure range up to ~ 0.4 GPa [5], which supports this idea. Here we review such novel phenomena observed in β-$YbAlB_4$ as well as those found in its isostructural polymorph α-$YbAlB_4$ discussing a possible role of valence fluctuation and anisotropic hybridization. In particular, we will discuss a sharp valence crossover induced by a chemical substitution in α-$YbAlB_4$ where we found a pronounced NFL behavior as a possible evidence of a quantum valence criticality [6]. These works have been done in collaboration with P. Coleman, A. H. Nevidomskyy, T. Sakakibara, Y. Uwatoko, Y. Karaki, K. Sone, J. Hong, S. Suzuki, H. Cao, D. MacLaughin, M. Okawa, Y. Takata, M. Matsunami, R. Eguchi, M. Taguchi, A Chainani, S. Shin, Y. Nishino, K. Tamasaku, M. Yabashi, T. Ishikawa, Y. Kiuchi, D. Hamane, M. Isobe, M. Koike. We thank them for their contributions.

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Classification of two-dimensional symmetry protected topological phases with a reflection symmetry

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After discovery of a topological crystalline insulator in SnTe[1,2], it became clear that spatial symmetries can protect topological structures. As well as this new phase, realization of topological phases is reported not only for free-fermion systems but also for correlated systems including spin and bosonic systems. Such phases are called as symmetry protected topological (SPT) phases. Employing a classification scheme based on the Chern-Simons theory[3,4], we classify SPT phases protected by a reflection symmetry. Besides, we propose a spin model which shows nontrivial phase protected by the reflection symmetry[5]. This is a bosonic extension of topological crystalline insulators. In study of femionic systems, we elucidate that correlation effects can reduce topological classification; topological classes in free fermion systems are reduced into those of Z_N in the presence of a local discrete symmetry. Here, N denotes order of the local symmetry.

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Quantum Fluctuations in Exchange-Based Spin Ice $Pr_2Zr_2O_7$

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Spin ice on pyrochlore lattice is a prototypical example of frustrated magnetism in which dipolar interactions between classical spins stabilize a frozen constrained state [1]. Remarkably, it exhibits a finite residual entropy resembling to the disordered proton configuration of water ice as well as emergent magnetic monopolar quasi-particles [2]. Recently, introducing quantum fluctuations into spin ice has attracted considerable interest because of the possible realization of novel quantum states, such as quantum spin liquid that exhibits quantum version of magnetic monopoles.

In this talk, we will present our recent results on a new class of spin ice material $Pr_2Zr_2O_7$, where spin correlations are provided by quantum mechanical superexchange interactions rather than classical dipolar interactions [3,4]. Similarly to conventional spin ice, magnetic susceptibility and specific heat show activated dynamics. Pinch-point features in quasi-elastic diffuse neutron scattering reflects adherence to a divergence free local constraint for disordered spins on long time scales. In sharp contrast to conventional ice, however, more than 90% of the neutron scattering is inelastic and devoid of pinch points furnishing evidence for magnetic monopolar quantum fluctuations. We will also present results of low-temperature properties under a magnetic field as well as systematic study on the relationship between low-temperature properties and sample quality.

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Magnetic monopoles in diluted quantum spin ice

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Quantum spin ice is a topic of much current interest, stemming from its promise as a topological spin liquid in $3d$, as well as recent discoveries of candidate compounds. However, precisely what signatures to look for to nail down quantum behavior in the spin ices is not clear. In this talk I will show that the most visible place to look for quantum effects in spin ice is in the presence of emergent magnetic monopoles, whose fractionalized nature is perhaps the most striking feature of this system.

Our focus is on the case of weakly diluted quantum spin ice, where we find the emergence of hydrogenic excited states, resembling those in doped semiconductors, in which a magnetic monopole is bound to a vacancy at various distances. We obtain an approximate expression for the dynamic neutron scattering structure factor [1] via a mapping to an effective exactly solvable model defined on the Bethe lattice.

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Dynamics of coupled electrons, skrymions and monopoles

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A swirling spin texture in magnets, skyrmion, is an emergent topological particle recently discovered in several chiral magnets, and is now recognized as a promising candidate for the information carrier in magnetic memories [1]. Furthermore, the creation (termination) point of a skyrmion corresponds to the monopole (anti-monopole) in three dimensional systems. The conduction electrons coupled to these topological spin textures show rich behaviors distinct from those in other situations.

We theoretically study the coupled dynamics of this system in terms of the numerical solution of Landau-Lifshitz-Gilbert equation, first-principles band structure calculations, and field theoretical methods. The topics include the quantized anomalous Hall effect in skyrmion crystal, resistivity induced by the monopole fluctuation, and current-driven motion of skyrmions.

Collaborators of these works are J. Iwasaki, W. Koshibae, Aron Beekman, M. Mostovoy, J.D. Zang, M. Mochizuki, J. H. Park, J. H. Han, C. Schuette, A. Rosch, X. Z. Yu, Y. Matsui, Y. Onose, N. Kanazawa, T. Ideue, Y. Shiomi, Y. Taguchi, and Y. Tokura.

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Light-induced Higgs-mode resonance in s-wave and d-wave superconductors

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Collective modes of the order parameter inherent in superconductors are classified into two: the phase and amplitude modes. The former corresponds to the Nambu-Goldstone (NG) mode, while the latter is often called the Higgs mode, in analogy with the recently discovered Higgs particle in high-energy physics. In superconductors, the NG mode is pushed to high energy ($\sim$ plasma frequency) due to the Anderson-Higgs mechanism, whereas the Higgs mode remains to exist in the low-energy regime. The extended BCS theory predicts that the Higgs-mode energy is given by 2Δ (i.e., the superconducting gap), so that the Higgs mode is the lowest energy excitation degenerate to the bottom energy of quasiparticle excitations. Since the Higgs mode is a scalar-boson excitation without being accompanied by quantum numbers such as electric charge, magnetic moment, etc., it has been difficult to excite and detect the Higgs mode by external perturbations in experiments.

Here we present how the Higgs mode can be coherently excited by strong laser fields for both s-wave and d-wave superconductors. For s-wave superconductors, we employ the Bogoliubov-de Gennes (BdG) equation and nonequilibrium dynamical mean-field theory [1] to show that an ac electric field with frequency Ω should induce a collective amplitude oscillation of the order parameter with a frequency 2Ω via the nonlinear light-matter coupling [2]. The induced oscillation turns out to become "resonant" with the Higgs mode when the resonance condition $2\Omega = 2\Delta$ is satisfied. This results in a giant third-harmonic generation (THG). One can distinguish the Higgs-mode resonance from quasiparticle excitations at the band-edge singularity by looking at the peak structure of the THG susceptibility. These phenomena have been recently observed in a THz laser experiment [3] in nice agreement with the theory. For d-wave superconductors, we calculate the susceptibility for the order-parameter oscillation induced by the ac field based on the mean-field theory, and find that the Higgs-mode resonance appears as a broad peak with 2Ω slightly smaller than $|2\Delta(\boldsymbol{k} = (\pi, 0))|$. This can be understood from the fact that the pairing interaction peaked at the antinode contributes to the Higgs-mode resonance.

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Solidifying a Quantum Spin Liquid in a 3D Toric Code

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While some extremely frustrated magnets may realize quantum spin liquids (QSLs), proposed frustrated quantum Hamiltonians are very difficult to deal with, and it is by no means easy to obtain conclusive evidence. On the other hand, a series of models such as the Kitaev model [1] and its extensions are useful in examining generic properties of QSLs, because it can be rigorously shown that their ground states are QSLs and moreover perturbative as well as thermal effects can be investigated at a quantitative level by using numerical methods. In this talk, I will present the thermodynamic phase diagram of a 3D toric code perturbed by ferromagnetic Ising interaction obtained by quantum Monte Carlo simulations. The interaction introduces quantum fluctuations to the loop-type "magnetic flux" excitations, which are confined at low temperature and responsible for stabilizing a QSL phase at finite temperature [2]. At a large enough value of this coupling, the interaction eventually "solidifies" the spin liquid into a magnetic ordered state breaking global Z_2 symmetry. We find that the critical temperature to the QSL phase is almost insensitive to the magnitude of the Ising coupling and also that the transition between the QSL and long-range ordered phases is strongly discontinuous. Near and inside the topological phase, we use the directed-loop algorithm supplemented by what we call "fictitious vertices," with which the multi-spin off-diagonal terms can be treated very efficiently.

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Dynamics of Quantum Spin-Liquids

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We provide a complete and exact theoretical study of the dynamical structure factor of a two-dimensional quantum spin liquid in gapless and gapped phases, as realized in Kitaevs honeycomb model. We show that there are direct signatures – qualitative and quantitative – of the Majorana fermions and gauge fluxes emerging in this model. These include counterintuitive manifestations of quantum number fractionalization, such as a neutron scattering response with a gap even in the presence of gapless excitations, and a sharp component despite the fractionalization of electron spin. Our analysis identifies new varieties of the venerable x-ray edge problem and explores connections to the physics of quantum quenches. I will present the results for the structure factor in 2D Kitaev honeycomb model and in its 3D (hyperhoneycomb lattice) generalization [3].

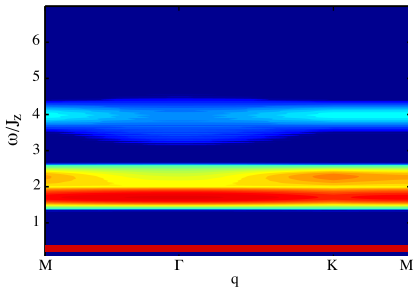

Figure 1: Dynamic structure factor in the gapped QSL phase of a 2D Kitaev honeycomb model on a logarithmic color scale [1] as a function of ω along the cut $\mathsf{M\Gamma KM}$ in the Brillouin zone. Remarkably the structure factor shows a sharp δ-function response (red bar at the bottom).

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Poster Presentations

PS-01

Periodically-driven Kondo impurity coupled to an ultracold fermionic bath

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The dynamics of a single impurity coupled to a fermionic or bosonic bath is one of the fundamental problems in condensed matter physics, and plays an important role in the polaronic systems, X-ray absorption problem, Kondo effect and so on. Recently, these impurity problems are studied in the ultracold atomic systems [1, 2, 3]. By utilizing their high controllability, nonequilibrium dynamics of impurity is also studied; for example, space- and time-resolved observation of a mobile spin impurity in a one-dimensional lattice system [3], Orthogonal Catastrophe by the radio-frequency field [4], and periodically driven spin-boson model [5].

In this paper, we study the periodically-driven impurity spin dynamics coupled to an ultracold fermionic bath by the Kondo exchange coupling. The time-dependent Hamiltonian we consider here is given by

$$H(t) = H_{Bath} + J_z S^z s^z(0) + J_\perp(t)(S^+\psi^\dagger_\downarrow(0)\psi_\uparrow(0) + h.c) + h(t)S^z \tag{1}$$

where H_{Bath} describes a one-dimensional fermionic bath, whose spin $s^z(x)$ at $x = 0$ is coupled to the impurity spin S^z via the anisotropic Kondo coupling J_z and $J_\perp(t)$. The time-dependent local magnetic field is denoted by $h(t)$.

In general, even in the noninteracting case, it is difficult to solve the dynamics of the periodically driven quantum system analytically. Thus we consider the case that the external field changes its values discretely in time and the Hamiltonian is at the special point in the parameter space (Toulouse limit) at which we can solve each time-step analytically and thereby treat the full dynamics exactly. Then, taking the continuum limit, we obtain a solution precisely for arbitrary time-periodic external fields.

We calculate the expectation values of the impurity spin and the magnetization of bath fermions in several different cases: (i) $h(t)$ has a rectangular-type time-dependence and $J_\perp(t)$ is time-independent, (ii) $h(t)$ has a sinusoidal time-dependence which is discretized appropriately and $J_\perp(t)$ is time-independent. As a result, we find that their characteristic behavior changes dramatically with the field-intensity h, the field-frequency Ω, and the Kondo temperature T_K. In $h \gg \Omega, T_K$, they oscillate with the frequency of h, while in $\Omega \gg h, T_K$, they approach a temporally constant value.

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PS-02

Photo-Induced Kondo Effect and its Anomalous Behavior

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Kondo effect is a ubiquitous phenomenon in condensed matter physics. It plays a key role in many systems such as heavy-fermion materials, leading to plethora of intriguing quantum phenomena. In this presentation, we propose a novel route to induce the Kondo effect, using *external laser excitation*. Naturally, it is tightly connected to non-equilibrium physics in condensed matter. We discuss here the realization scheme of the photo-induced Kondo effect, and its anomalous properties in the non-equilibrium steady state.

Our scheme is motivated by recent development of manipulation techniques in ultracold atomic gases [1-4]. Using ultracold fermions with two orbitals and optical transition between them, effective hybridization between orbitals is induced, which results in the emergence of the Kondo effect. The heavy-fermion liquid realized by the laser shows intriguing behavior, since the laser field strongly couples with the spin degrees of freedom. We demonstrate that the laser-induced Kondo state leads to component-selective renormalization of effective masses, and also show that novel competition with other Kondo screening channels drives a photo-induced "switch" of the Kondo effect.

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PS-03

Transport properties for a quantum dot coupled to normal leads with the pseudogap structure

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Magnetic impurity problems in d-wave superconductors or Dirac fermions have been discussed in the context of the pseudogap Kondo problem [1,2]. Recently, quantum dot systems coupled to normal leads with the pseudogap structure have attracted much attention [3]. In the equilibrium system, the competition between the Kondo and local moment states has been discussed in detail [1,2]. By contrast, in the non-equilibrium system with a finite voltage, the systematic analysis is lacking, and thereby it is necessary to study how the pseudogap structure affects the transport properties in the quantum dot system.

In this study, we consider a symmetric pseudogap Anderson impurity model as

$$\hat{H} = \sum_{\sigma} \varepsilon_d \hat{n}_{d\sigma} + \sum_{k\sigma\alpha} (\varepsilon_k - \mu_\alpha) \hat{n}_{k\sigma\alpha} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{k\sigma\alpha} \left(v \hat{c}^{\dagger}_{k\sigma\alpha} \hat{d}_{\sigma} + \text{H.c.} \right), \tag{1}$$

where $\hat{c}_{k\sigma\alpha}$ is the annihilation operator of an electron with wave number k and spin $\sigma(=\uparrow,\downarrow)$ in the αth lead, and $\hat{n}_{k\sigma\alpha} = \hat{c}^{\dagger}_{k\sigma\alpha} \hat{c}_{k\sigma\alpha}$. $\hat{d}_{\sigma}$ is the annihilation operator of an electron at the quantum dot, $\hat{n}_{\sigma} = \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma}$. ε_k is the dispersion relation of the lead and v is the hybridization between the lead and quantum dot. ϵ_d and U are the energy level and Coulomb interaction at the quantum dot. To discuss how the pseudogap structure affects steady state properties, we consider the density of states for both leads $\rho_\alpha(\omega) = \rho_0 |\omega|^r$, where r is the pseudogap parameter. We then set the chemical potentials as $\mu_1 = V/2$ and $\mu_2 = -V/2$, where V is the bias voltage. Applying the second-order perturbation theory [4,5] to the model, we clarify that the pseudogap structure in the normal leads induces the cusp structure in the density of states, in addition to the Coulomb peaks. The r-dependence of the conductance is also addressed.

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PS-04

Dynamical mean-field analysis of non-equilibrium relaxation processes in an electron-phonon coupled system

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The non-equilibrium properties of correlated systems have recently attracted a lot of interest because of cold-atom and pump-probe experiments. In the non-equilibrium dynamics of solids, electron-phonon (e-ph) interactions are expected to play an important role. From a microscopic and theoretical point of view, fundamental properties of electron-phonon systems can be captured by the simple Holstein model. However, many non-equilibrium properties of this model have yet to be revealed. Here, in order to obtain new insights of non-equilibrium physics in e-ph systems, we investigate the Holstein model both in the normal and superconducting states with the non-equilibrium dynamical mean-field theory (DMFT) [1].

In the normal state and in the weak-coupling regime, a crossover from electron- to phonon-dominated relaxation is observed when the electron-phonon coupling is changed [2]. Namely, in the weaker-coupling regime, oscillations in physical quantities decay before the momentum distribution of the electrons approaches its thermal value, while in the stronger-coupling regime, the electron momentum distribution approaches a thermal value before the oscillations are damped. We show that this crossover originates from the different dependence of the electron and phonon self-energies on the e-ph coupling.

In the superconducting state [3], both the phonon mode and the collective amplitude (Higgs) mode of the superconducting order parameter show up in the relaxation process. We reveal that the phonon mode becomes long-lived when the e-ph coupling is sufficiently strong, which leads to qualitatively different relaxation processes at weak and strong coupling. This behavior in the time domain turns out to be related to properties of the spectral functions of electrons and phonons. We also discuss possibility of non-thermal critical points in this model, where the superconductivity is long-lived beyond its phase boundary in equilibrium.

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PS-05

Phase diagram of a one-dimensional generalized cluster model and dynamics during an interaction sweep

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We study quantum phase transitions and dynamical properties in the one-dimensional cluster model with several interactions

$$H_{\mathrm{GC}} = \sum_{i=1}^{N} (-J^{XZX} \sigma_i^x \sigma_{i+1}^z \sigma_{i+2}^x + J^{YY} \sigma_i^y \sigma_{i+1}^y + J^{YZY} \sigma_i^y \sigma_{i+1}^z \sigma_{i+2}^y) \tag{1}$$

using exact diagonalization and infinite Time Evolving Block Decimation (iTEBD). First, the ground-state phase diagram of the model is determined and each phase is characterized by order parameters. We confirm that the degeneracy of the lowest levels in entanglement spectrum corresponds to that of the ground state in the model with open boundary condition. Second, we investigate dynamical properties during an interaction sweep through the critical points of the model with open boundary condition using the time-dependent Bogoliubov transformation. After passing the critical point, a periodic structure in the length dependence of correlation functions and entanglement entropy is observed, which stems from the Bogoliubov excitations generated near the critical points.

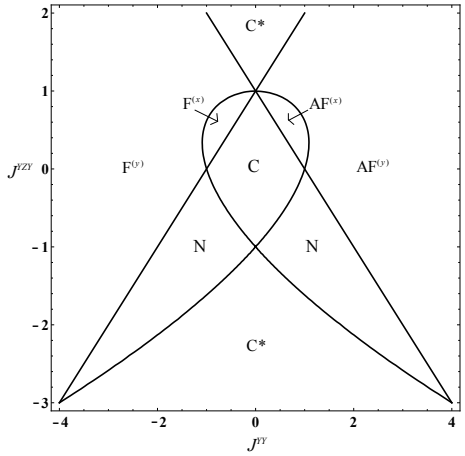

Figure 1: Phase diagram of the generalized cluster model (1) with $J^{XZX} = 1$. The excitation gap vanishes on the solid curves. C, C*, F, and AF represent cluster, dual cluster, ferromagnetic, and antiferromagnetic phases, respectively. The N phase cannot be characterized by string and (anti) ferromagnetic order parameters. The superscript represents the direction of the order. Each phase is determined by order parameters calculated with exact diagonalization and iTEBD.

PS-06

Flux quench in the $S = 1/2$ XXZ chain

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We study a *flux quench* problem in the spin-1/2 XXZ chain. The flux quench is a quantum quench where the flux ϕ piercing the XXZ chain is turned off at $t = 0$ suddenly. If we formulate the XXZ chain as a spinless fermion model, the flux ϕ corresponds to a vector potential on each bond and this flux quench can be viewed as imposing a pulse (delta function) of electric field. Therefore some particle (or spin) current is generated in the system at $t = 0$. Recently this quench was studied to illustrate the breakdown of the generalized Gibbs ensemble in integrable systems [1]. Here, we focus on the time-evolution of the spin current after the quench and calculate it numerically by the infinite time-evolving block decimation (iTEBD) method.

We find that the dynamics of the spin current depends strongly on the anisotropy parameter Δ of the XXZ chain and the amount of flux initially inserted. The long-time limit ($t \to \infty$) of the current matches with predictions of linear response theory as the initial flux decreases, but the deviation from linear response theory is largely affected by the sign of interactions. Furthermore, in some parameter region the current oscillates in time (Fig. 1, left panel) and the frequency of the oscillation is proportional to $|\Delta|$. Remarkably, the dynamics of momentum distribution of the spinless fermions reveals that this oscillation of the current is governed by excitations deep inside the shifted Fermi sea (Fig. 1, right panel). This mechanism of oscillations cannot be captured by the effective Luttinger model corresponding to the microscopic XXZ chain, which is in contrast with the previous studies on different types of quench in the same model [2].

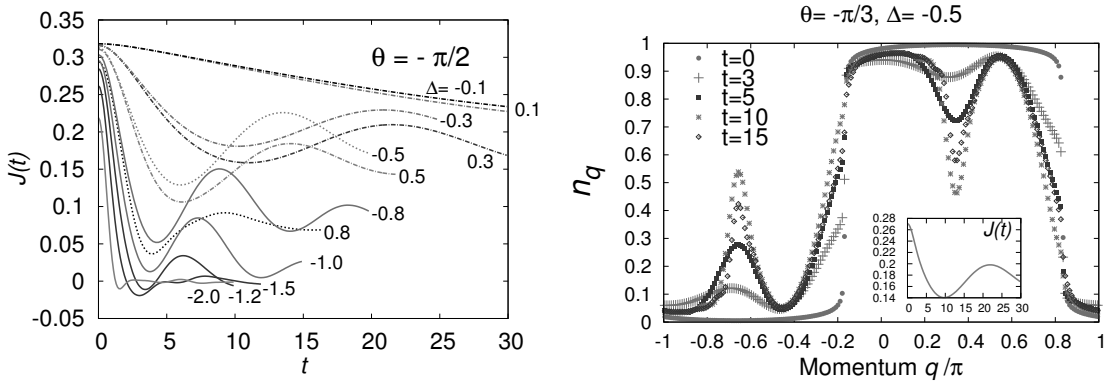

Figure 1: Left: Dynamics of the spin current after the quench. θ is initial flux per site. Anisotropy Δ is defined as $H_{\mathrm{XXZ}} = -\sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right)$. Right: momentum distribution of the spinless fermions. The dip (peak) structure deep inside the shifted Fermi sea is observed (the inset shows the time-evolution of the current).

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PS-07

Topological Kondo insulators in strong laser fields

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Controlling the nature of matter by laser light is an important topic in strongly correlated electron systems. We theoretically investigated how high-frequency laser field changes the nature of topological Kondo insulators. The topological Kondo insulator is a strongly correlated insulator that has a surface state protected by time-reversal symmetry (TRS) [1]. Recent theoretical and experimental studies suggest that SmB_6 is a strong candidate for the topological Kondo insulator.

By employing a prototypical model of the topological Kondo insulator [2], we treated the effect of laser field with the effective Floquet Hamiltonian, which gives the information of the system in the high-frequency limit. It enables us to map the time-periodic systems to static systems. We treated electron correlation effects by the slave-boson method, which allows us to calculate the renormalization effect self-consistently and thus determine the Kondo temperature.

From the topological point of view, we showed how the laser light changes the topological phases of this system. We calculated the topological number at the mean field level and found how topological phase transitions occur according to laser intensity. Especially when the light is circularly polarized, TRS is broken. In that case we showed that the system is driven to a quantum Hall phase and a Weyl semi-metallic phase.

In terms of the heavy fermion physics, we calculated the Kondo temperature as a function of laser light intensity and discussed the intensity-temperature phase diagram. Our calculation elucidated that there are the photo-induced hopping and the photo-induced hybridization under the laser irradiation, and that these photo-induced effects change the nature of the heavy electrons in the system quantitatively.

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PS-08

Effect of Ca-Doping on Pyrochlore Iridates $Nd_2Ir_2O_7$

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Pyrochlore iridates $Ln_2Ir_2O_7$ (*Ln* = Nd - Ho) exhibit metal-insulator transitions (MITs) [1, 2]. The 4*f* electrons from Ln^{3+} are well localized. As the $(5d)^5$ electrons from Ir^{4+} form an unfilled t_{2g} band, the 5*d* electrons contribute to the electrical conductivity. Their electrical conductivity and transition temperatures (T_{MI}) depend on the ionic radius of Ln^{3+}: the resistivity at room temperature and T_{MI} increase with a reduction in the ionic radius. This fact means that the origin of MITs comes from Ir 5*d* electrons. In addition, these MITs involve an antiferromagnetic magnetic ordering of Ir moment with all-in/all-out arrangement [3-5]. Recent theoretical study predicts a new antiferromagnetic QCP around the disappearance of MIT [6]. In order to the criticality of this MIT, we have investigated the carrier doping effect. In this presentation, we will report the Ca-doping effect in $Nd_2Ir_2O_7$ (T_{MI} =33 K). Figure 1 shows the electrical resistivity of $(Na_{1-x}Ca_x)_2Ir_2O_7$. The MIT is rapidly suppressed with Ca-doping; T_{MI} = 12 K for x = 0.05. Finally, the MIT disappears at x =0.15. We will also shows the experimental results of magnetization, specific heat, thermoelectric power, and high-field magnetoresistance effect in this presentation.

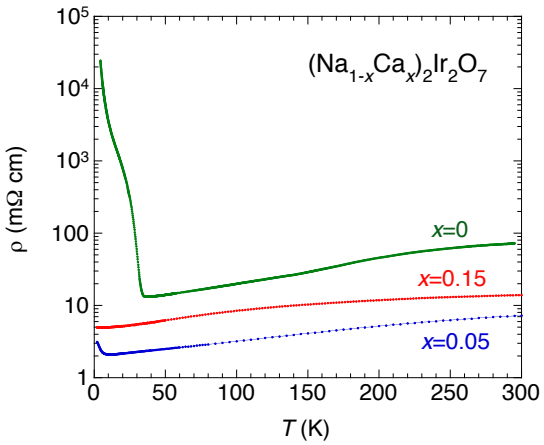

Fig.1. Electrical resistivity of $(Na_{1-x}Ca_x)_2Ir_2O_7$.

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PS-09

Dynamical analyses of condensed-phase hydrogens using nuclear and electron wave packet molecular dynamics simulation

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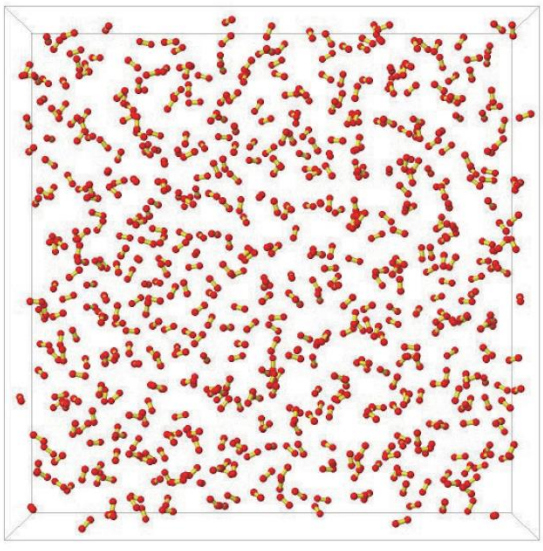
Understanding microscopic dynamics of condensed-phase systems exhibiting strong quantum effects is still one of the important open problems. Hydrogen is of primary importance not only in the fundamental condensed phase physics but also in its potential applications as energy source without harmful byproducts. Although hydrogen is the simplest of all molecular species, nuclear quantum effects (NQEs) dominate properties of the condensed phases.

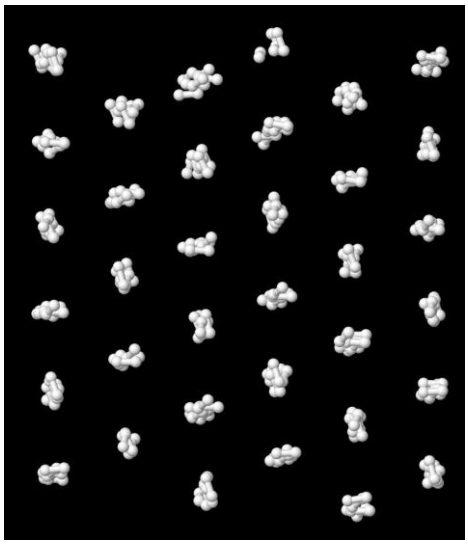
We recently proposed the real-time simulation method of nuclear and electron wave packet molecular dynamics (NEWPMD) based on the non-empirical intra- and inter-molecular interactions.[1,2,3] This is the first time that the real-time quantum molecular dynamics simulation without any model potentials for hydrogen interactions is developed and applied to condensed-phase hydrogens taking into account the NQEs such as nuclear delocalization and zero-point energy.

In the proposed method, the NQEs are non-perturbatively taken into account. Any electronic model potentials for hydrogen interactions including the intra- and inter-molecular energies of non-spherical hydrogen molecules do not need to be given in advance since all electrons are explicitly treated by fermionic EWPs to account for their correlations. Nevertheless, its computational cost is quite reasonable.

Liquid para-hydrogen (p-H_2) typically exhibits the strong NQEs and thus anomalous static and dynamical properties at low temperature. We confirmed that the NEWPMD successfully reproduces the experimental basic properties of p-H_2 liquid such as radial distribution functions, self-diffusion coefficients, and shear viscosities, demonstrating that the NEWPMD can be a powerful and efficient quantum MD simulation method to study nonequilibrium and dynamical processes of condensed-phase hydrogens. Our recent project on dynamical analyses of solid p-H_2 will be also mentioned in my presentation. These studies open a new area of hydrogen material research to understand anomalous quantum properties which are difficult to be accessible by use of conventional MD simulation techniques as well as usual density functional theories which generally lack a long-range dispersion force.



Dynamics snapshot of Liquid p-H_2 at 25 K



Dynamics snapshot of Solid p-H_2 at 2.5 K

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PS-10

First Principle Calculation of Electronic Structures of Lanthanide Oxides with Pseudopotential Method

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First principle determination of electronic structures of strongly correlated electronic systems (SCESs) is a subject of substantial concern in solid state physics and electronic structure theory. The electronic structure of SCESs is known to be calculated by the density functional+U (DFT+U) method treating correlated electrons as real electrons and itinerant electrons as DFT electrons. Empirical *U* parameters are usually used for describing the on-site interaction between the correlated electrons, however, use of empirical *U* parameters tarnishes the statues of the method and lowers its calculation accuracy. In this study, we introduced the first principles DFT+U pseudopotential (DFT+U PP) method, which is free from any empirical parameters, and applied it to the electronic structure calculation of lanthanide oxides having correlated electrons. Our method is based on a fact that the DFT energy of a material is proportional to Un^2, where n is the number of correlated electrons on the atom of the material. This method is an extension of the constraint DFT method introduced by McMahan *et al*.[1] for the linearized muffin-thin (LMTO) method. Our DFT+U calculations provided insulating electronic structures for lanthanide oxides, reproducing an experimental fact that they are insulating, in contrast to the conventional DFT PP calculation, which provided metallic electronic structures for them, as shown for Ce_2O_3 in Figure 1.

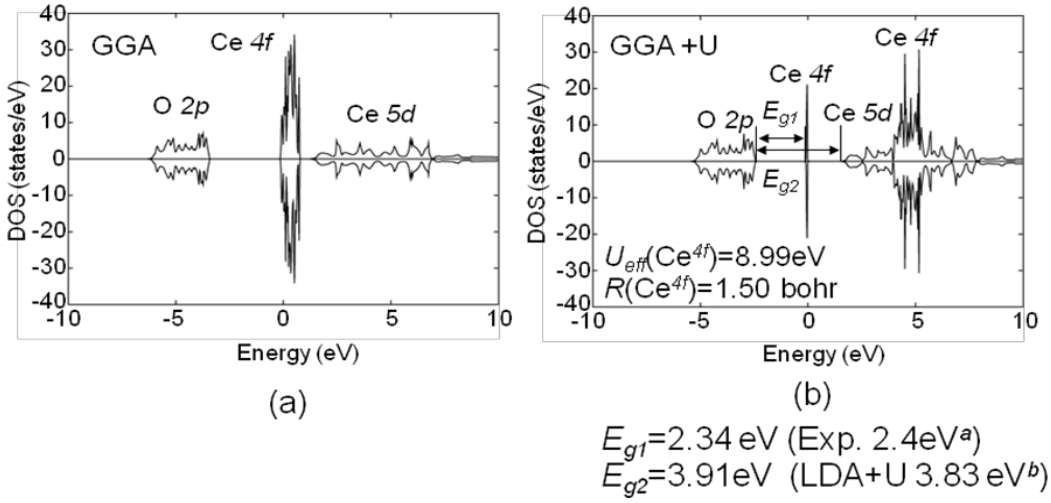

Fig. 1 Electronic density of states of Ce_2O_3 in the antiferromagnetic state: (a) GGA PP and (b) GGA+U PP calculation results.

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PS-11

Fano resonance between Higgs bound states and Nambu-Goldstone modes

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Stimulated by the recent report of observing the Higgs boson in elementary particle physics, the studies of the Higgs modes have attracted a lot of attention in condensed matter physics. Up to the present, many efforts have been made to observe the Higgs modes in various condensed matter systems, such as quantum dimer antiferromagnets [1], superconductors [2], charge-density-wave materials [3], superfluid ^{3}He-B phase [4], and ultra-cold Bose gases in optical lattices [5,6]. Thanks to an approximate particle-hole symmetry, these systems are nearly Lorentz-invariant [7] so that the Higgs mode emerges.

We study collective modes of superfluid Bose gases in optical lattices combined with potential barriers. Bose gases in a sufficiently deep optical lattice are described by Bose-Hubbard (BH) model. We assume that the system is in the vicinity of the quantum phase transition to a Mott insulator at a commensurate filling, and analyze the collective modes with the time-dependent Ginzburg Landau (TDGL) equation [8] which is microscopically derived from BH model. In a homogeneous system, an emergent particle-hole symmetry gives rise to two types of collective mode: gapless Nambu-Goldstone (NG) mode and gapful Higgs mode [9]. Here, we consider two kinds of potential barrier: one shifts the chemical potential that breaks the particle-hole symmetry, and the other changes the hopping amplitude that holds the particle-hole symmetry. In the presence of the latter barrier, we find bound states of the Higgs modes called *Higgs bound states* that have binding energies lower than the bulk Higgs gap and are localized around the barrier. We show that the former barrier couples the Higgs bound states with the NG mode such that the NG mode incident to the barriers can exhibit Fano resonance mediated by the bound states.

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PS-12

Convergence for the Groundstate Auxiliary Field method

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For small Hubbard-clusters for which the numerical diagonalization results are known, we show that for the groundstate auxiliary field method, the Monte-Carlo convergence of the energy is consistent with self-averaging quantities $1/\sqrt{LN}$ (Number of sites L, number of Monte-Carlo samples N_s), not only to $1/\sqrt{N}$ as for non-self-averaging quantities. We also discuss the final error as obtained by the corresponding error in the Suzuki-Trotter decomposition and the effect the sign has on the convergence.

PS-13

Theoretical Study of Charge-Spin-Orbital Fluctuations in Mixed Valence Spinels: AlV_2O_4 and LiV_2O_4

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We theoretically investigate the fluctuations in charge, spin, and orbital degrees of freedom in spinel oxides AB_2O_4. We are particularly interested in mixed valence compounds, in which the nominal number of d electrons at the B cation is not an integer. As the B cations comprise a pyrochlore lattice as shown in Fig. 1, the mixed valence spinels are a good playground for the interplay of multiple degrees of freedom on the geometrically frustrated lattice structure. In the present study, we focus on two spinels, AlV_2O_4 and LiV_2O_4, which show puzzling, contrasting behavior despite the common structure: AlV_2O_4 exhibits a peculiar structural phase transition with a self-organization of seven V clusters (heptamers) at 700 K [1], while LiV_2O_4 does not show any transition down to the lowest temperature except for crossover to an unconventional heavy fermion state at 20-30 K [2]. In order to clarify the origin of the contrasting behavior, we adopt the combined method between the first-principles calculation and the perturbation in terms of electron correlations. Specifically, we construct the multiband Hubbard model by the maximally-localized Wannier function analysis for the LDA band structure. We then calculate the generalized susceptibility, which includes all the information of fluctuations in charge, spin, and orbital sectors, by incorporating the electron correlations at the level of the random phase approximation.

For AlV_2O_4, we find that the dominant fluctuations appear in the vicinity of the Γ point in the Brillouin zone. Although there are many eigenmodes entangled with each other, we unveil that peculiar charge fluctuations are sensitively enhanced by the inter-site Coulomb interaction. The enhanced fluctuations are of σ-bonding type with strong orbital dependence, as schematically shown in Fig. 2. The importance of similar σ-bonding states in the hepmater formation was suggested in the previous experimental and theoretical studies [1,3]. Hence, our results provide a key for understanding of the self-organization in AlV_2O_4. In contrast, for LiV_2O_4, we find that the sixteen eigenmodes related to a_{1g} orbital have relatively larger eigenvalues and well separated from other modes even in the non-interacting case. We show that the on-site interaction enhances the optical-type spin fluctuations at an incommensurate wave number, as schematically shown in Fig. 3. In this fluctuation, the net spin fluctuation vanishes in the four-site tetrahedron. This fluctuation is enhanced at very low temperature, in the order of 10 K, which is suggestive of the peculiar heavy fermion behavior in LiV_2O_4.

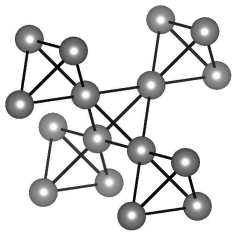

Fig. 1: Pyrochlore lattice.

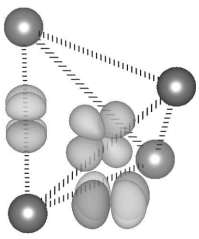

Fig. 2: σ-bonding fluctuation in AlV_2O_4.

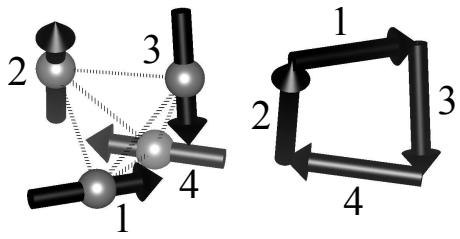

Fig. 3: Optical-type spin fluctuation in LiV_2O_4.

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PS-14

Excitonic Multipole Order in a *d-p* Model with Parity Mixing

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Multipole orders have attracted much attention in condensed matter physics, as they lead to exotic electronic, transport, and optical properties. For instance, the multipole orders induced by the strong spin-orbit coupling and electron correlation have been extensively studied in various *f*-electron materials [1]. Recently, unconventional multipole orders associated with conventional electronic symmetry breaking have also been of great interests. A typical example is found in several pyrochlore compounds, such as Os and Ir pyrochlores [2-4]. In these compounds, a noncoplanar all-in/all-out type magnetic (dipole) order was discussed as a magnetic octupole order, which leads to unconventional phenomena [5]. Similar multipole orders (magnetic toroidal and quadrupole orders) were discussed theoretically on a zigzag chain [6,7] and a honeycomb lattice [8-11], paying attention to the effects of the atomic spin-orbit coupling and the mixing of different parity orbitals. In these previous works, however, multipole orders always appear subsidiary to the lower-rank electronic orders. It is important to explore the possibility of pure, primary multipole ordering for deeper understanding of the multipole physics. In particular, it will be interesting to explore yet another type of multipole orders for further exotic phenomena beyond those in *f*-electron systems.

In order to search such primary multipole orders, we consider a simple *d-p* model on a zigzag chain, which incorporates the spin-orbit coupling and the parity mixing. The model is considered as an extension of the multi-orbital model discussed for excitonic orders [12]. Using the Hartree-Fock approximation, we obtain the ground-state phase diagram of this model at half filling in a wide range of intra and interorbital Coulomb interactions. The result shows that a pure multipole ordered phase appears as an intermediate phase between the band insulating phase with the *d-p* hybridization gap and the antiferromagnetic phase caused by the strong intraorbital Coulomb interaction. The intermediate phase has a magnetic quadrupole order with an excitonic nature from the orbital mixing, which is stabilized by the spin-orbit coupling and the parity mixing. We also find that the multipole ordered phase exhibits a peculiar band deformation with a shift of the band bottom in the momentum space in an applied magnetic field.

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PS-15

Finite Temperature Phase Transition in Chiral Spin Liquids

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Quantum spin liquid (QSL) is an exotic quantum state of matter in insulating magnets, where long-range ordering is suppressed down to the lowest temperature (T). Among many possible realizations of QSLs, the chiral spin liquid, in which the time reversal symmetry is broken, has attracted considerable interest in not only condensed matter physics but also quantum information. This is because its excitation is suggested to be a non-Abelian anyon that works as an operator in topological quantum computing [1]. For exploring the possibility of quantum computing, it is important to clarify how thermal fluctuations act on the chiral spin liquids and their excitations.

In the present study, in order to reveal the thermodynamic properties in chiral spin liquids, we address the Kitaev model on the decorated honeycomb lattice depicted in Fig. 1. The ground state properties of this model were originally predicted by A. Kitaev [1], and studied in detail by the exact solution by H. Yao and S. Kivelson [2]. The model exhibits two different types of the chiral spin liquids accompanied with non-Abelian and Abelian anyons in the ground state. These two phases appear by changing the exchange parameters J and J' for intra- and inter-triangles, respectively. Here, we investigate the finite-T properties in this extended Kitaev model by using the quantum Monte Carlo simulation in the Majorana representation that we developed [3,4]. We find that the model exhibits the finite-T phase transition associated with time reversal symmetry breaking. In the case of $J' \gg J$, we show that the phase transition is of second order. This result is confirmed by a Monte Carlo simulation in the effective model in the limit of $J' \gg J$: we show that the transition belongs to the two-dimensional Ising universality class. With decreasing J'/J, however, the phase transition is changed to first order, indicating the existence of the tricritical point in the phase diagram. Moreover, we calculate the Chern number and the thermal Hall conductivity. In the parameter region where the non-Abelian anyon excitation is expected, we find that these quantities become nonzero below T_c due to the edge current of itinerant Majorana fermions.

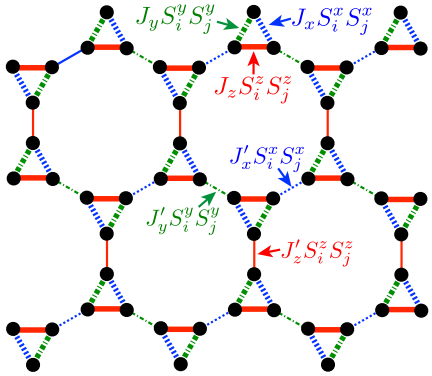

Figure 1: Schematic picture of a two-dimensional decorated honeycomb lattice. In the Kitaev model defined on this lattice, the interactions on the dashed, dashed-and-dotted, and solid bonds are of Ising type with only the x, y, and z spin components, respectively. In the present calculations, we impose $J = J_x = J_y = J_z$ (bold lines) and $J' = J'_x = J'_y = J'_z$ (thin lines).

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PS-16

Magnetization Process in a Frustrated Spin Ladder

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Recently, a cascade of phase transitions induced by magnetic field has been observed in $BiCu_2PO_6$ [1,2], whose effective spin model, a frustrated two-leg spin ladder, bridges between the frustrated spin chain and the non-frustrated spin ladder with one-half spins [2,3]. According to the theoretical studies, the zigzag spin chain exhibits one-third plateau [4], although no plateau emerges in the non-frustrated spin ladder [5]. Therefore, the simple question arises as to whether plateaux do appear in the frustrated spin ladder, or not. To clarify the question, we calculate rung-coupling dependence and frustration dependence of magnetization process by using density-matrix renormalization-group method. In this calculation, we find some plateaux at m=1/2 and 2/3, which do not appear in both the frustrated spin chain and the non-frustrated spin ladder, in addition to 1/3 plateau and some cusps [6]. We analytically find out a correspondence between effective models in weak and strong rung-coupling limits, which gives an explanation of the plateaux and cusps.

Our study is useful to analyze experimental data of $BiCu_2PO_6$.

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PS-17

Topological quantum phase transition in an SU(N)-invariant spin chain

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In traditional condensed-matter physics, high symmetry like SU(N) is realized in rather idealized situations and has been used mainly as mathematical convenience. Recently, SU(N)-symmetric fermion systems were realized using alkaline-earth atoms loaded in optical lattices [1,2]. Since a variety of novel quantum phases are expected [3], theoretical understanding of quantum phases in the SU(N) fermion systems is urgent. We focus on the Mott phase with N fermions per site in one dimension where the effective Hamiltonian is described by the SU(N) Heisenberg spin chain. Generally, gapped (bosonic) phases with SU(N)-symmetry are classified into one trivial and $N-1$ nontrivial topological classes [4]. With the entanglement spectrum [5], we found for $N=4$ that the ground state of the above SU(N) Heisenberg model is in one of these (symmetry-protected) topological phases [6].

In this presentation, we consider a variant of the SU(4) Heisenberg Hamiltonian with quadratic and cubic terms to investigate a quantum phase transition out of the topological phase. Using infinite Time-Evolving Block Decimation (iTEBD) method [7], we obtained the ground state, which is then characterized by the structure of low-lying entanglement spectrum. As a result, there is a topological-non-topological quantum phase transition between the SU(4) VBS and the dimer phases. We also determined the transition point using the string and the dimer order parameters.

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PS-18

Meron Crystals with Spin Scalar Chiral Stripes

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Chiral magnets with noncoplanar spin structures, e.g., skyrmion crystals, have drawn a lot of attention for their peculiar transport phenomena and a wide variety of potential applications [1]. In these systems, the spin scalar chirality defined by the triple product of three spins plays an essential role because it acts as an effective magnetic field for electrons via the spin Berry phase mechanism. In fact, there have been several studies on spin-charge coupled systems, focusing on a ferroic spin scalar chiral ordering [2, 3, 4, 5]. Recently, a spatially-modulated spin scalar chiral ordering also draws considerable interest, as it might lead to a rich variety of novel electronic structures and transport phenomena [6]. However, the determination of precise magnetic structure requires considerable effort, since the chiral ordered state sometimes has quite a large magnetic unit cell, which is hard to treat numerically.

In this study, in order to explore such intriguing possibility of spatially−modulated chiral orders, we focus on multiple-Q orderings characterized by more than one wave vector, anticipated from the instability of Fermi surface [4, 7, 8]. Specifically, we consider the Kondo lattice model with the nearest- (t_1) and third-neighbor (t_3) hoppings on a square lattice. In this model, while tuning t_1 and t_3, the dispersion relation has four saddle points at the Lifshitz transition point. These saddle points give rise to the van Hove singularity in the density of states. Such singular behavior is expected to enhance the instability of the Fermi surface. We calculate the low-temperature properties of the model by performing the efficient numerical simulation based on the Langevin dynamics for localized spins with the kernel polynomial method [9]. As a result, we show that spin scalar chiral stripes accompanied with double-Q ordering emerge around the Lifshitz transition point. Surprisingly, the obtained stripes are regarded as a crystal of peculiar spin textures called merons (half of the skyrmions) [10]. We also investigate the stabilizing mechanism by the analytical perturbation approach with respect to the spin-charge coupling as well as the numerical variational calculations for the ground state. We discuss transport properties induced by the novel spin scalar chiral stripes.

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Chiral magnetic effect in insulators

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Using the topological insulator multilayer[1] model originally proposed as a model of Weyl semimetal we discuss the possible realization of chiral magnetic effect in insulators. For parameters giving an insulating phase, we calculated chiral magnetic conductivity of the model using the standard Kubo formula. Although the previous study[2] based on a formation of landau levels implied that in the insulating phase chiral magnetic conductivity becomes zero, we found that this is an artifact of the unbounded linear dispersion corresponding to the surface state dispersion of the topological insulator layers. Indeed, we could obtain a nonzero result by introducing a cutoff Λ which is physically a bulk energy gap of these topological insulator layers. Moreover, we constructed the model which realizes nonzero chiral magnetic effect and has completely periodic momentum space(BZ).

To uncover the role of the energy gap for chiral magnetic effect, we calculated finite frequency chiral magnetic conductivity of a massive Dirac model with a finite chiral chemical potential, which is known as the minimal insulating model realizing chiral magnetic effect. We found that the effect is rather enhanced for $\omega \neq 0$ by the energy gap. This is because the presence of the energy gap protects the system from low energy excitations which are the source of the characteristic discontinuity observed in the massless case[3] that reduces the low frequency response to one third of $\omega = 0$ one.

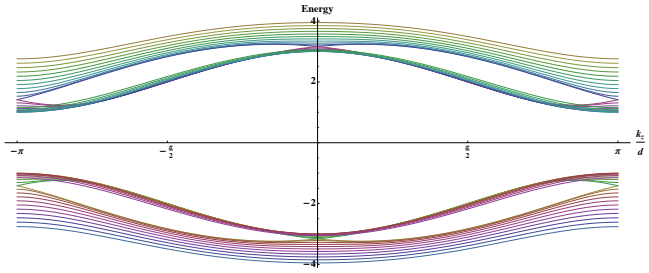

Figure 1: Energy dispersion of the multilayer model with parameters realizing an insulating phase.

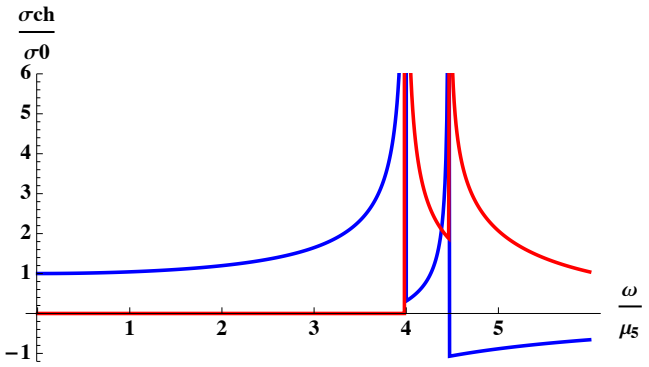

Figure 2: Frequency dependence of chiral magnetic effect of the massive Dirac model. Blue: Real part, Red: Imaginary part.

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